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NUMERICAL SOLUTION OF A COMBUSTION MODEL WITH THERMAL CONDUCTIVITY AND REACTANT DIFFUSIVITY IN ARBITRARY DOMAINS USING THE VARIATIONAL ITERATION METHOD

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DEDICATED TO PROFESSOR ADEWALE ROLAND TUNDE SOLARIN ON THE OCCASION OF HIS 70TH BIRTHDAY

ABSTRACT. This paper presents the numerical solution of a combustion model with thermal conductivity and reactant diffusivity in arbitrary domains using the Variational Iteration Method (VIM). The paper begins with a brief introduction of the model and the basic idea of VIM. This is followed by the numerical solutions of the model and animated graphical representation of the solutions. The result obtained demonstrates that the model is highly sensitive to initial conditions, and its applicability is dependent on thermal conductivity and reactant diffusivity values. Computations are carried out using Maple 18 software.

1. INTRODUCTION

We consider the following strongly coupled quasilinear parabolic combustion model with thermal conductivity and reactant diffusivity in non-smooth domains presented by Sanni [1] of the form:

$$\frac{\partial u}{\partial t} - div(\phi \nabla u) = Qwf(u), \qquad in \quad \Omega \times [0,\infty) \tag{1}$$

$$\frac{\partial w}{\partial t} - div(\Psi \nabla w) = wf(u), \qquad in \quad \Omega \times [0,\infty) \tag{2}$$

$$\frac{\partial u}{\partial \mathbf{n}} = \frac{\partial w}{\partial \mathbf{n}} = 0 \qquad on \quad \partial\Omega \times [0,\infty) \tag{3}$$

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$$u(x,0) = u_0(x), w(x,0) = w_0(x) \tag{4}$$

Where

$$\phi = h^1(x,t,u,w), \Psi = h^2(x,t,u,w) \tag{5}$$

Here $Qwf(u)$ and $-wf(u)$ are the reaction Kinetics determined by a positive, uniformly bounded, differentiable Lipschitz continuous function $f(u).f'(u)$ is also assumed to be Lipschitz continuous.

The system (1)-(4) represents a one-step irreversible reaction, reactant$\rightarrow$ product. $w(x,t)$ is assumed to be the mass fraction of the reactant, $1-w(x,t)$, the mass fraction of the product, $u(x,t)$ the temperature in the reaction vessel, $\phi(x,t,u,w)$ the thermal conductivity, and $\Psi(x,t,u,w)$ the reactant diffusivity [1].

We remark that combustion modeling indeed has a rich history in mathematical research. However, as stated by Buckmaster [2], making useful contribution to combustion requires an extensive apprenticeship in the relevant physics. The work of Buckmaster et al. [3] and the references therein provides much on the fundamentals of combustion. Interestingly, equations derived for combustion processes may find usefulness in other areas. One fascinating example of such an equation is the Kuramoto-Sivashinsky Equation (KSE). Originally proposed by Kuramoto [4] and independently by Sivashinsky [5] to model flame front instability and phase turbulence in chemical reactions, the KSE has found applications in reaction-diffusion systems, flame propagation, thin hydrodynamic films, and viscous flow problems [6], [7]. Whether or not the system (1) – (4) finds usefulness in other areas besides combustion will be subject of other studies.

The existence of a unique, global and strong solution to the system (1)-(4) was proven in [1]. Fitzgibbon and Martin [8], presented an extensive discussion of the quasilinear parabolic combustion model and solutions to variants of (1)-(4) using the Forward-Euler Finite difference scheme. In this study, we apply He's [9], [10] Variational Iteration Method (VIM) to finding the numerical solution to the system (1)-(4). The basic idea of the method is summarized below:

Consider the following nonlinear differential equation:

$$Lu + Nu = g(x) \tag{6}$$

Where L is a linear operator, N is a nonlinear operator and $g(x)$ is a known function. VIM presents a correction functional for equation (6) in the form:

$$u_{n+1}(x) = u_n(x) + \int_0^x \lambda(s)(Lu_n(s) + N\widetilde{u}_n(s) - g(s))ds \qquad (7)$$

Where $\lambda(s)$ is a general Lagrange's multiplier, which may be a constant or a function, and may be identified optimally via variational theory [11],[12]. The subscript n denotes the nth approximation, and $\widetilde{u}_n$is considered a restricted variation i.e. $\partial\widetilde{u}_n = 0$. The langrage multiplier $\lambda(s)$ in (7) is accurately determined using calculus of variation and variational theories. Accurate or approximate Lagrange multiplier for the scheme may also be determined using the formula:

$$\lambda(s) = \frac{(-1)^n}{(n-1)!}(s-x)^{n-1} \qquad (8)$$

Upon the determination of the Lagrange multiplier $\lambda(s)$, we determine the iteration formula as:

$$u_{n+1}(x) = u_n(x) + \frac{(-1)^n}{(n-1)!}\int_0^x (s-x)^(n-1)(Lu_n(s) + N\widetilde{u}_n(s) - g(s))ds \qquad (9)$$

A preferred zeroth approximation is selected, and other iterations follow. Several studies [13], [14], [15] [16] have shown that VIM is able to solve systems of linear and non-linear partial differential equations.

2. . NUMERICAL APPLICATION

PROBLEM 1

To solve (1)-(4), we re-write (1) and (2) in the form:

$$\frac{\partial u}{\partial t} - \left(\phi\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x}\frac{\partial \phi}{\partial x}\right) = wf(u) \qquad (10)$$

$$\frac{\partial w}{\partial t} - \left(\Psi\frac{\partial^2 w}{\partial x^2} + \frac{\partial w}{\partial x}\frac{\partial \phi}{\partial x}\right) = -wf(u) \qquad (11)$$

And assume the following initial conditions,

$$u(x,0) = tanh(3x^2 + x), w(x,0) = tanh(3x+5) \qquad (12)$$

The thermal conductivity, and reactant diffusivity are assumed to be of the respective forms:

$$\phi = u(x,t)e^{(2x^3+4x^2+x)} - w(x,t), \Psi = u(x,t)\alpha e^{(x^2+x)} - w(x,t) \qquad (13)$$

$$f(u) = \beta e^u \lambda > 0, \alpha > 0, \beta > 0 \qquad (14)$$

Furthermore, we shall solve the problem for

$$\beta = \lambda = \alpha = 1 \tag{15}$$

We assume that time t is measure in seconds and the reactant and byproduct are assigned appropriate measurement in grams or Kilogram as the case maybe.

Solution

To solve the model (10)-(14), we construct two correction functionals of the form:

$$u_{n+1}(x,t) = u_n(x,t) + \int_0^x \lambda_1(s)\Bigg(\frac{\partial u(x,s)}{\partial s} - \left(\phi\frac{\partial^2 u(x,s)}{\partial x^2} + \frac{\partial u(x,s)}{\partial x}\frac{\partial \phi}{\partial x}\right) - w(x,t)f(u(x,s))\Bigg)ds \tag{16}$$

$$w_{n+1}(x,t) = w_n(x,t) + \int_0^x \lambda_2(s)\Bigg(\frac{\partial w(x,s)}{\partial s} - \Bigg(\Psi\frac{\partial^2 w(x,s)}{\partial x^2} + \frac{\partial w(x,s)}{\partial x}\frac{\partial \phi}{\partial x}\Bigg) + w(x,t)f(u(x,s))\Bigg)ds \tag{17}$$

$$We \quad determine \quad \lambda_1(s) = \lambda_2(s) = -1 \tag{18}$$

So that we get the following iteration formula:

$$u_{n+1}(x,t) = u_n(x,t) - \int_0^x \left(\frac{\partial u(x,s)}{\partial s} - \left(\phi\frac{\partial^2 u(x,s)}{\partial x^2} + \frac{\partial u(x,s)}{\partial x}\frac{\partial \phi}{\partial x}\right) - w(x,t)f(u(x,s))\right)ds \tag{19}$$

$$w_{n+1}(x,t) = w_n(x,t) - \int_0^x \left(\frac{\partial w(x,s)}{\partial s} - \left(\Psi\frac{\partial^2 w(x,s)}{\partial x^2} + \frac{\partial w(x,s)}{\partial x}\frac{\partial \phi}{\partial x}\right) + w(x,t)f(u(x,s))\right)ds \tag{20}$$

We determine the zeroth (initial) approximation as:

$$u_0(x,t) = u(x,0) = tanh(3x^2 + x), w_0(x,t) = w(x,0) = tanh(3x+5) \tag{21}$$

Using the iteration formulas (19) and (20) and the zeroth approximations (21), we determine the following iterations:

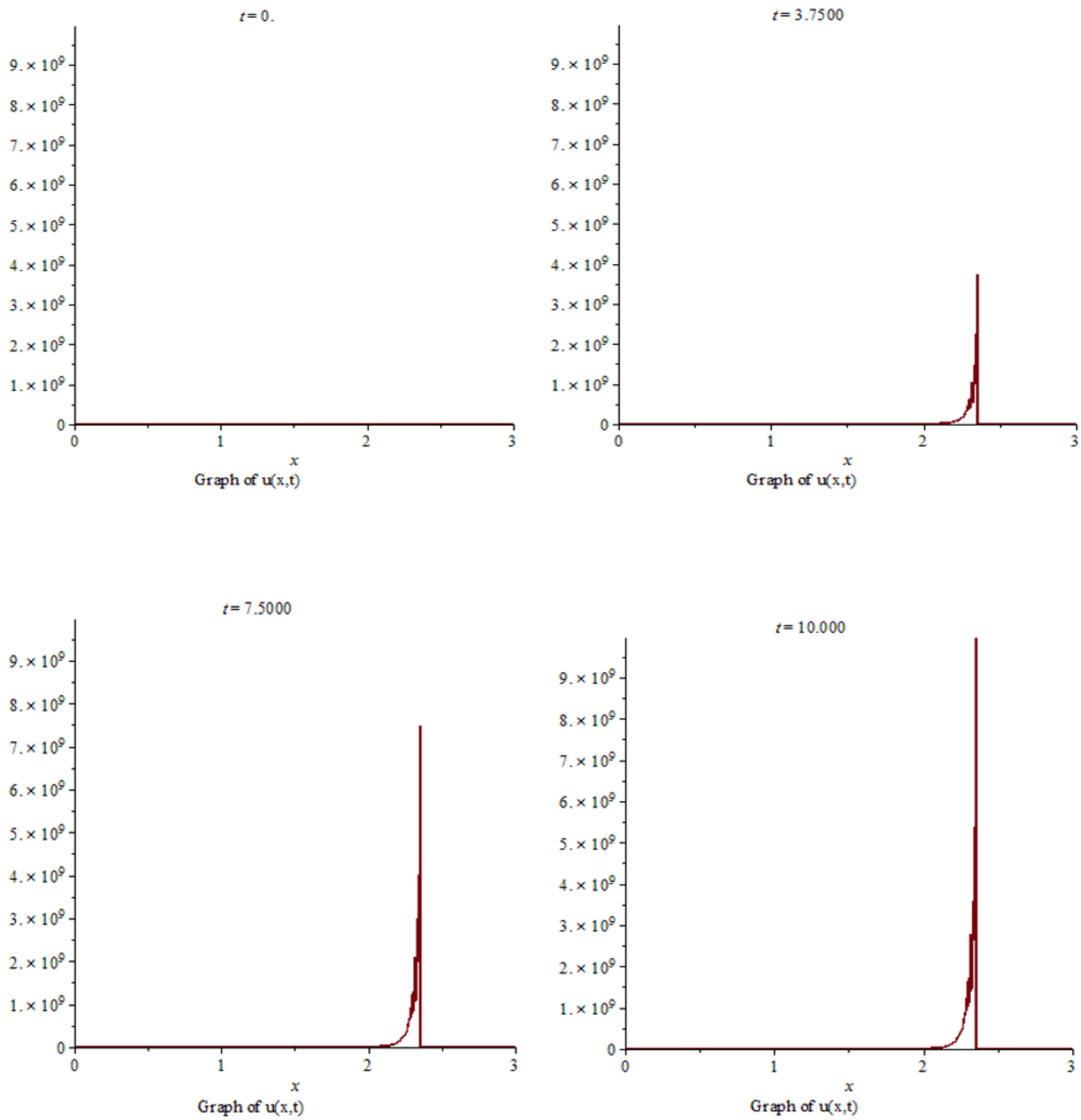
$$
\begin{aligned}
u_1(x,t) = tanh(3x^2+x) + \Big(tanh(3x^2+x)e^{2x^3+4x^2+x} - tanh(3x+5)\Big) \\
\Big(-2tanh(3x^2+x)\Big(1-tanh(3x^2+x)^2\Big)(6x+1)^2 + 6 - 6tanh(3x^2+x)^2\Big)t \\
+\Big(1-tanh(3x^2+x)^2\Big)(6x+1)\Big(\Big(1-tanh(3x^2+x)^2\Big)(6x+1)e^{2x^3+4x^2+x} \\
+tanh(3x^2+x)(6x^2+8x+1)e^{2x^3+4x^2+x} - 3 + 3tanh(3x+5)^2\Big)t \\
-tanh(3x+5)e^{tanh(3x^2+x)}t
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
w_1(x,t) = tanh(3x+5) - 6\Big(tanh(3x^2+x)e^{x2+x} - tanh(3x+5)\Big) \\
tanh(3x+5)\Big(3-3tanh(3x+5)^2\Big)t + \Big(3-3tanh(3x+5)^2\Big) \\
\Big(\Big(1-tanh(3x^2+x)^2\Big)(6x+1)e^{2x^3+4x^2+x} + tanh(3x^2+x)(6x^2+8x+1) \\
e^{2x^3+4x^2+x} - 3 + 3tanh(3x+5)^2\Big)t + tanh(3x+5)e^{tanh(3x^2+x)}t
\end{aligned}
\tag{23}
$$

$\cdots$ and so on.

We plot the result of the temperature $u_1(x,t)$ in the reaction vessel in Fig. 1-4 below:

Fig. 1-4: Depicting rising temperature $u(x,t)$ as time t progresses



PROBLEM 2

We repeat the process for the problem (10) - (15), using the following initial approximation:

$$u_0(x,t) = u(x,0) = tanh(3x^2 - 2x), w_0(x,t) = w(x,0) = tanh(3x+10) \tag{24}$$

The thermal conductivity and reactant diffusivity are assumed to be of the respective forms:

$$\phi = u(x,t)e^{(2x^3+4x^2+x)} - w(x,t), \Psi = u(x,t)\alpha e^{(x^2+x)} - w(x,t) \tag{25}$$

Solution

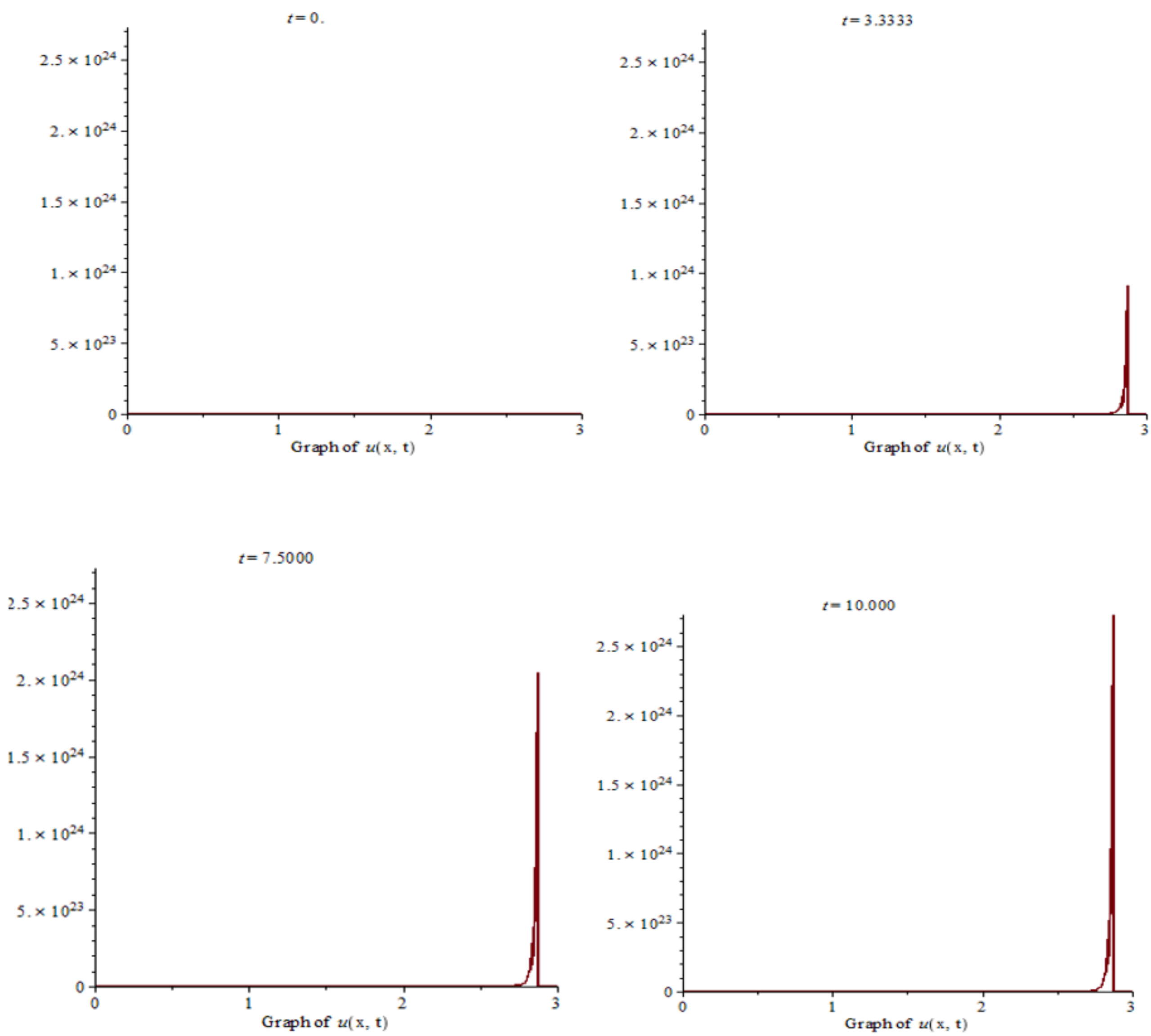
$$\begin{aligned} u_1(x,t) = {} & tanh(3x^2-2x) + \Big(tanh(3x^2-2x)e^{2x^3+4x^2+x} - tanh(3x+10)\Big) \\ & \Big(-2tanh(3x^2-2x)\Big(1-tanh(3x^2-2x)^2\Big)(6x-2)^2 + 6 - 6tanh(3x^2-2x)^2\Big)t \\ & + \Big(1-tanh(3x^2-2x)^2\Big)(6x-2)\Big(\Big(1-tanh(3x^2-2x)^2\Big) \\ & (6x-2)e^{2x^3+4x^2+x} + tanh(3x^2-2x)(6x^2+8x+1)e^{2x^3+4x^2+x} \\ & -3+3tanh(3x+10)^2\Big)t - tanh(3x+10)e^{tanh(3x^2-2x)}t \end{aligned} \tag{26}$$

$$\begin{aligned} w_1(x,t) = {} & tanh(3x+10) - 6\Big(tanh(3x^2-2x)e^{x^2+x} - tanh(3x+10)\Big)tanh(3x+1) \\ & \Big(3-3tanh(3x+10)^2\Big)t + \Big(3-3tanh(3x+10)^2\Big)\Big(\Big(1-tanh(3x^2-2x)^2\Big) \\ & (6x-2)e^{2x^3+4x^2+x} + tanh(3x^2-2x)(6x^2+8x+1)e^{2x^3+4x^2+x} - 3 \\ & + 3tanh(3x+10)^2\Big)t + tanh(3x+10)e^{tanh(3x^2-2x)}t \end{aligned} \tag{27}$$

$\cdots$ and so on.

We plot the result of the temperature $u_1(x,t)$ in the reaction vessel in Fig. 5-8 below

Fig. 5-8: Depicting rising temperature $u(x,t)$ over time t



The solutions $u(x,t)$, graphically illustrated in Fig 1- 4 for problem 1 and Fig. 5 – 8 for problem 2 depicts rising temperature of a combustion process over a period of time t. The ignition temperature for the combustion process is at time $t = 0$. We observe a steady rise of the flame like profiles of $u(x,t)$ as time t progresses for both problems considered. We note also that a small change to the initial conditions for problem 2, resulted in a change in height and a slight shift to the right of $u(x,t)$, despite using the same thermal conductivity and reactant diffusivity values for both problems. This indicates that the model is highly sensitive to initial conditions.

3. CONCLUSION

In this study, the Variational Iteration Method have been applied to finding the numerical solutions of the combustion model (1)-(5) using carefully chosen Zeroth approximation, thermal conductivity and reactant diffusivity in arbitrary domain with the results graphically illustrated and interpreted. It was demonstrated that VIM is able to give a straight forward handling of the model once the zeroth approximation, reactant diffusivity and thermal conductivity had been appropriately chosen in arbitrary domain. Choosing values for the zeroth approximation, reactant diffusivity and thermal conductivity in arbitrary domain to get interpretable results for the model can however be quite tricky and requires proper understanding of the fundamentals of the model. We remark that the model is able to yield a good number of interpretable numerical solutions depending on appropriately chosen zeroth approximation, thermal conductivity and reactant diffusivity.

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